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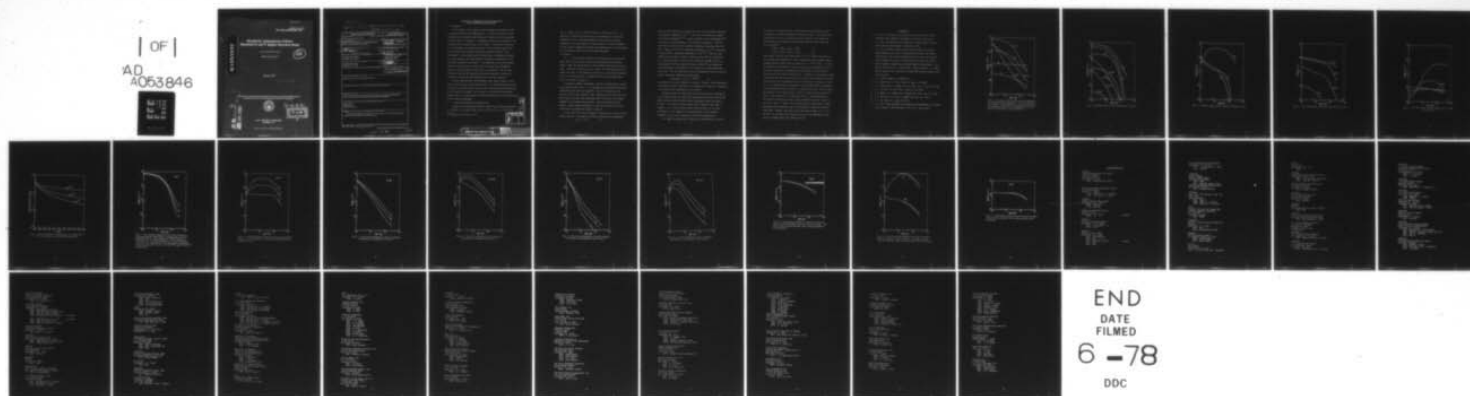
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# Sensitivity Assessments of Some Disturbed E and F Region Reaction Rates

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*Plasma Physics Division*

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February 1978

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# SENSITIVITY ASSESSMENTS OF SOME DISTURBED E AND F REGION REACTION RATES

## I Introduction

The disturbed E and F regions of the ionosphere play important roles on systems, detectors and communications. To assess the impact of such an environment, a detailed understanding of the physics and the chemistry of these regions is essential. An important aspect of this problem is the ionization and the deionization of the regions. These depend critically on a large number of reactions that occur in the disturbed region which in turn control and determine the extent, duration and decay of the disturbance. The ionization and the deionization is generally described by a time dependent code which monitors the density distributions of the disturbed ionospheric constituents. The complexity of such codes depend heavily on their utility in conjunction with large scale hydrodynamic codes, the desired output and the speed of calculation. Two NRL Codes, The Master Code and the Simple Code have been developed<sup>1</sup> to assess the ionization, deionization and radiation from the E and F regions.

The more detailed code, the NRL Master Code, remains dynamic in the sense of utilizing up-to-date reaction rates. It can be utilized to assess the impact of various reaction rates on the ionization and the deionization of the E and the F regions. In this report, we utilize the current NRL Master Code<sup>2</sup> for the assessment of several reaction rates on the deionization of the disturbed atmosphere.

## II A Brief Description of the Master Code

The Master Code calculates the time histories of the following species;  
 $N_2$ ,  $N_2(A^3\Sigma)$ ,  $O_2$ ,  $O_2(a^1\Delta)$ ,  $O_2(b^1\Sigma)$ ,  $NO$ ,  $O$ ,  $O(^1D)$ ,  $O(^1S)$ ,  $N$ ,  $N(^2D)$ ,  $N(^2P)$ ,

Note: Manuscript submitted January 31, 1978.

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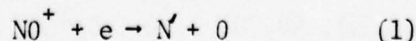
$N_2^+$ ,  $O_2^+$ ,  $O_2^+(a^4\pi)$ ,  $NO^+$ ,  $O^+$ ,  $O^+(^2D)$ ,  $O^+(^2P)$ ,  $N^+$ ,  $N^+(^1D)$  and  $N^+(^1S)$ . In addition, the Master Code calculates three temperatures; the electron temperature, the  $N_2$  vibrational temperature and the heavy particle temperature. The time histories of these species, the electron density and the relevant temperatures provide the ingredients for the calculations of the radiation emitted from the disturbed atmosphere.

### III Results

Six sets of initial conditions were chosen and the current NRL Master Code<sup>2</sup> was utilized to carry out the deionization calculations. Figure 1 shows the time histories of the electron densities for these six cases. Selecting a special case, e.g. Case I, the time histories of the atomic ions (Fig. 2), the molecular ions (Fig. 3), the atomic metastables (Fig. 4), and the densities of  $O_2(a^1\Delta)$ ,  $NO$  and the three temperatures (Fig. 4) are shown in Figures 2-5.

In keeping a general code dynamic, one must incorporate most current and reliable reaction rates. This procedure has been applied continuously to NRL Master Code from its inception<sup>3</sup>. Many of the reaction rates relevant to the E and F regions of the ionosphere and are utilized in NRL Master Code, have been well established under the reaction rate support program<sup>4</sup> of the Defense Nuclear Agency. Some of the reaction rates, however, require further experiments so that their values will be well established over temperature ranges of interest.

In this report we assess the impact of certain reaction rates on the electron density. For example, consider the dissociative recombination



where the rate coefficient utilized previously in the NRL Master Code had a temperature dependence of  $T_e^{-1.2}$ . This value was obtained by Biondi<sup>5</sup> from several measurements<sup>6,7,8</sup>. However, recently two new measurements<sup>9,10</sup> of reaction (1) have been made in two different experiments. These two experiments give two entirely different temperature dependences for the rate. Huang, et al<sup>9</sup>, give a temperature dependence of  $T_e^{-0.37}$  while Walls and Dunn obtain a temperature dependence of  $(T_e)^{-0.83}$ . These two rate coefficients are shown in Figure 6 along with the old<sup>5</sup> rate coefficient. It is seen from Figure 6 that the rate coefficient of Huang, et al<sup>9</sup> is large compared with that measured by Walls and Dunn<sup>10</sup>, even though the last measurement is undoubtedly for  $\text{NO}^+$  being in its ground vibrational state ( $V=0$ ). The rate coefficient with its dependence on both the electron and the vibrational temperature should follow

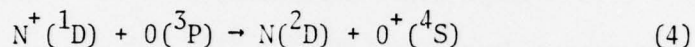
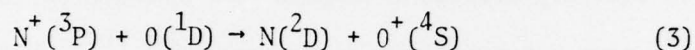
$$\text{Coefficient} \sim T_e^{-1/2} (1 - e^{h\nu/T_v}) \quad (2)$$

which makes the two rates somewhat of a puzzle. However, recent theoretical calculations by Lee<sup>11</sup>, attributes the discrepancy as being due to resonances in the dissociative recombination cross section.

Using the three rate coefficients for the dissociative recombination of  $\text{NO}^+$  shown in Figure 6, sensitivity calculations were made using the NRL Master Code for three different initial conditions indicated as Cases I, IV and V. The results for the electron and  $\text{NO}^+$  densities are shown in Figures 7-12. It can be stated clearly that the impact of this rate coefficient is very important on the deionization of the disturbed atmosphere, and as such on detection systems and communications.

In a highly disturbed E and F region, the concentrations of excited

metastables are appreciable, and a large number of near resonance charge exchange and ion-atom rearrangement reactions may occur. The reaction rate coefficients for most of these reactions are not known. We selected the following two near resonance charge exchange processes from a large set given elsewhere<sup>12</sup>



and assumed a reaction rate coefficient of  $5 \times 10^{-11} \text{ cm}^3/\text{sec}$  for each one. This assumed rate coefficient is small compared with near resonance charge exchange processes which are of the order of  $\sim 3 \times 10^{-10} \text{ cm}^3/\text{sec}$ . To assess the importance of reactions (3) and (4), a given initial condition, Case II, was used in sensitivity calculations and the results of certain species concentrations are shown in Figures 13-15. In Figure 13, the electron density calculations with and without reactions (3) and (4) are shown where the lower curve presents the electron density with the inclusion of reactions (3) and (4). It is apparent that the divergence in the electron density calculated with and without reactions (3) and (4), increases with time. The fast decay of electrons (lower curves of Figs. 3 and 4) is due to the conversion of  $\text{N}^+$  into  $\text{O}^+$ , which forms  $\text{NO}^+$  in its reaction with  $\text{N}_2$ . The corresponding  $\text{NO}$ ,  $\text{NO}^+$  and  $\text{N}(\text{}^2\text{D})$  densities are shown, with and without reactions (3) and (4), in Figs. 14 and 15. Clearly, if one raises the rate coefficient to higher and perhaps more reasonable values, the divergence in densities would be much higher. However, even with a rate coefficient as small as  $5 \times 10^{-11} \text{ cm}^3/\text{sec}$ , one can assess that reactions (3) and (4) are important at late-times for communications and infrared emission.



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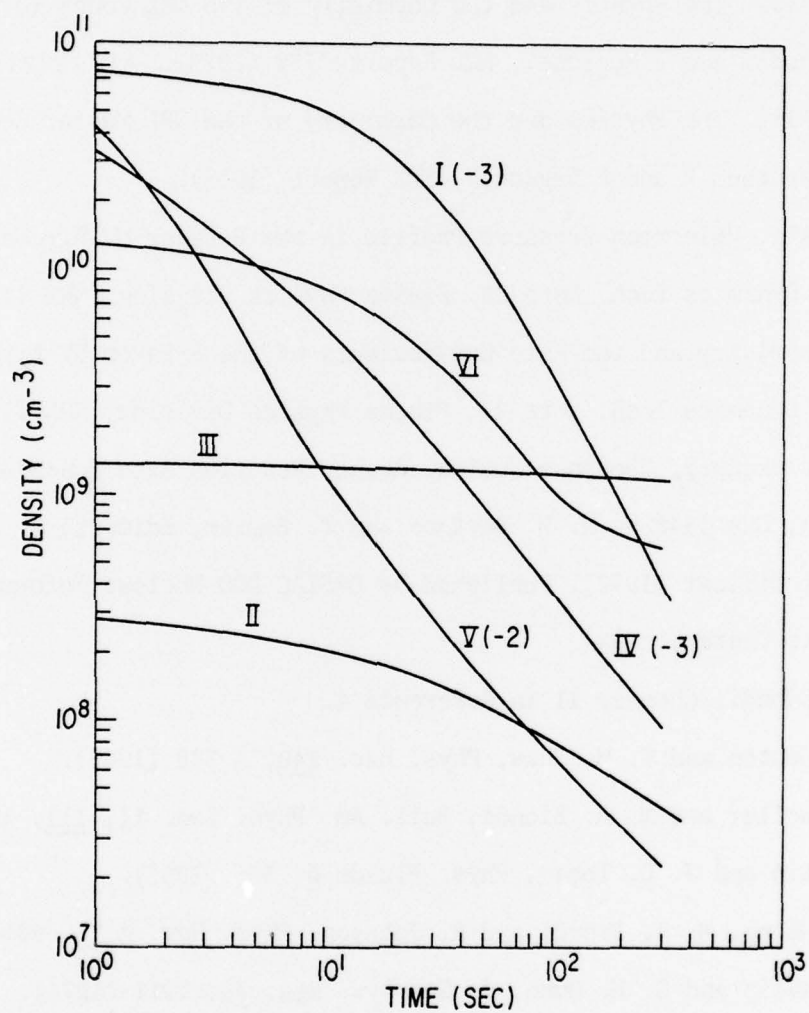


Fig. 1 - The time history of the electron density for six different initial conditions. For cases followed by a number in parenthesis, the electron density for the respective case is to be multiplied by 10 to the power of the number in the parenthesis.



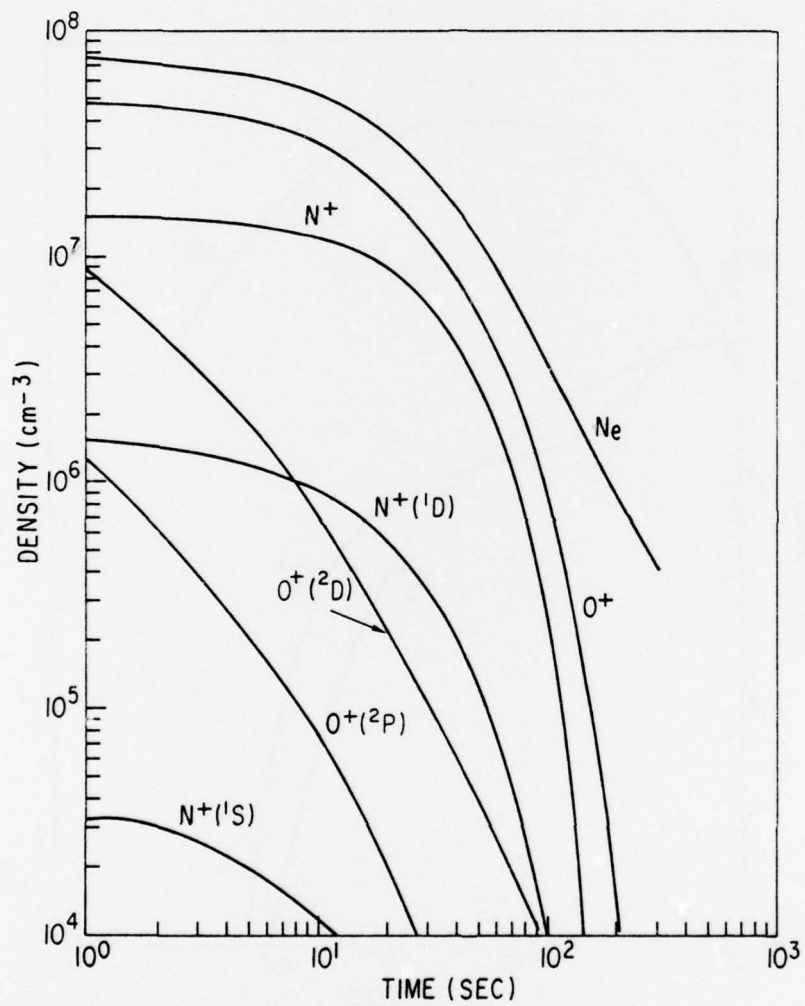


Fig. 2 - The time history of the atomic ions for Case I

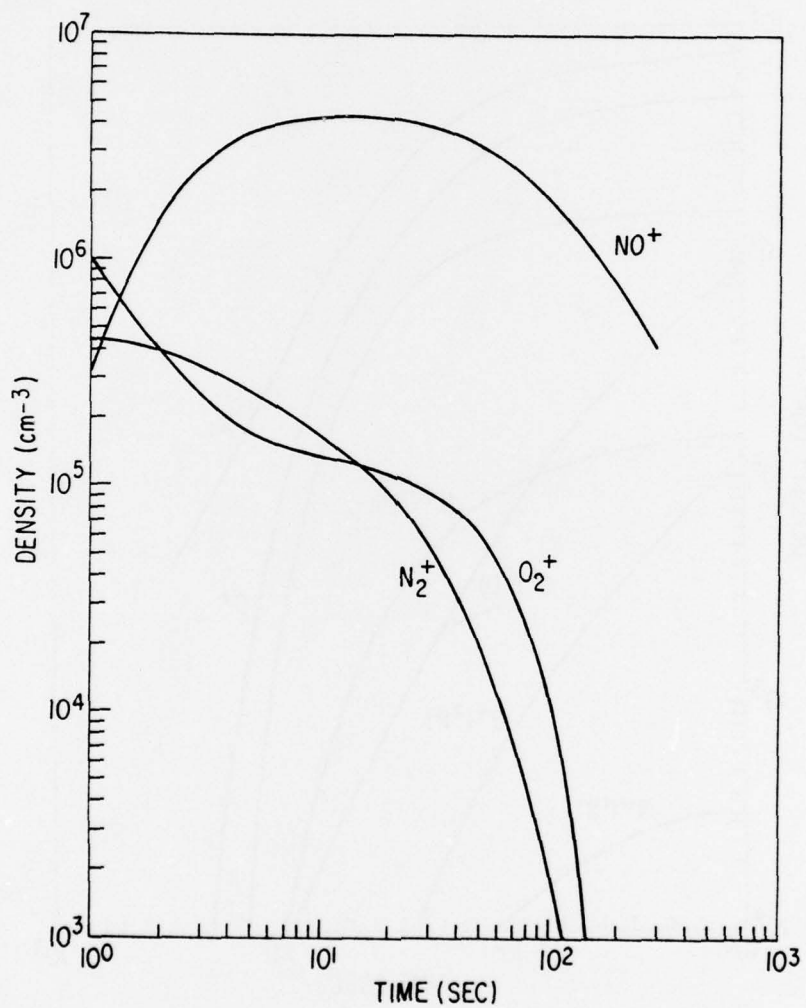


Fig. 3 - The time history of the molecular ions for Case I

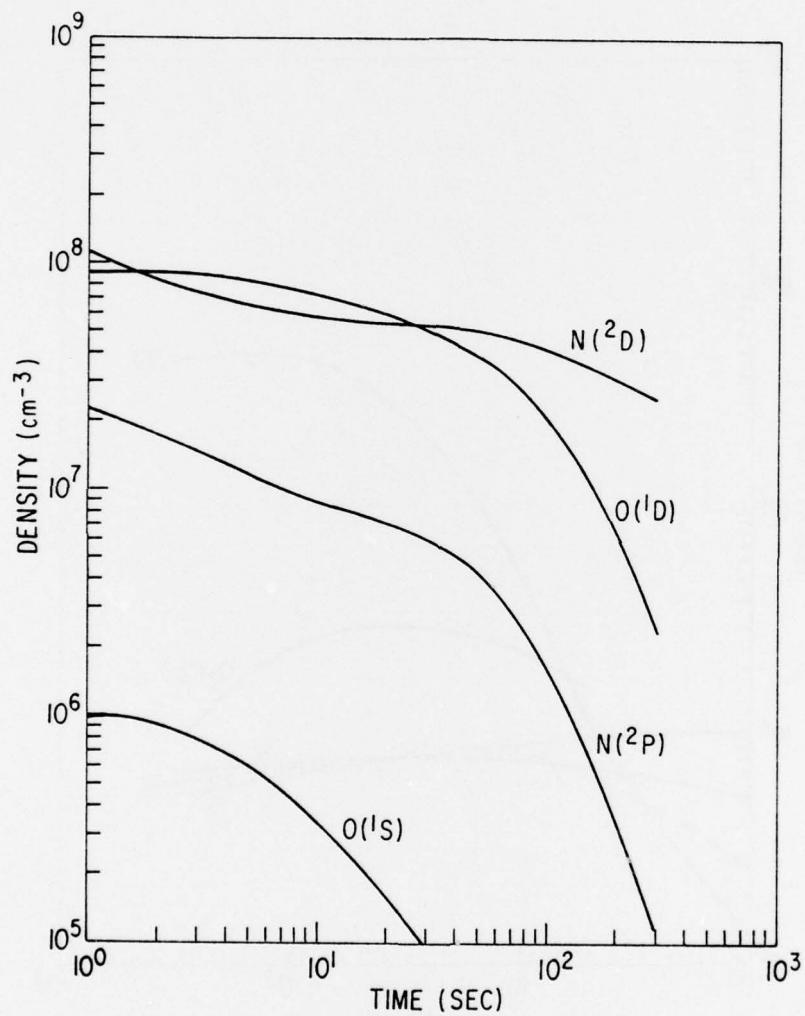


Fig. 4 - The time history of atomic metastables for Case I

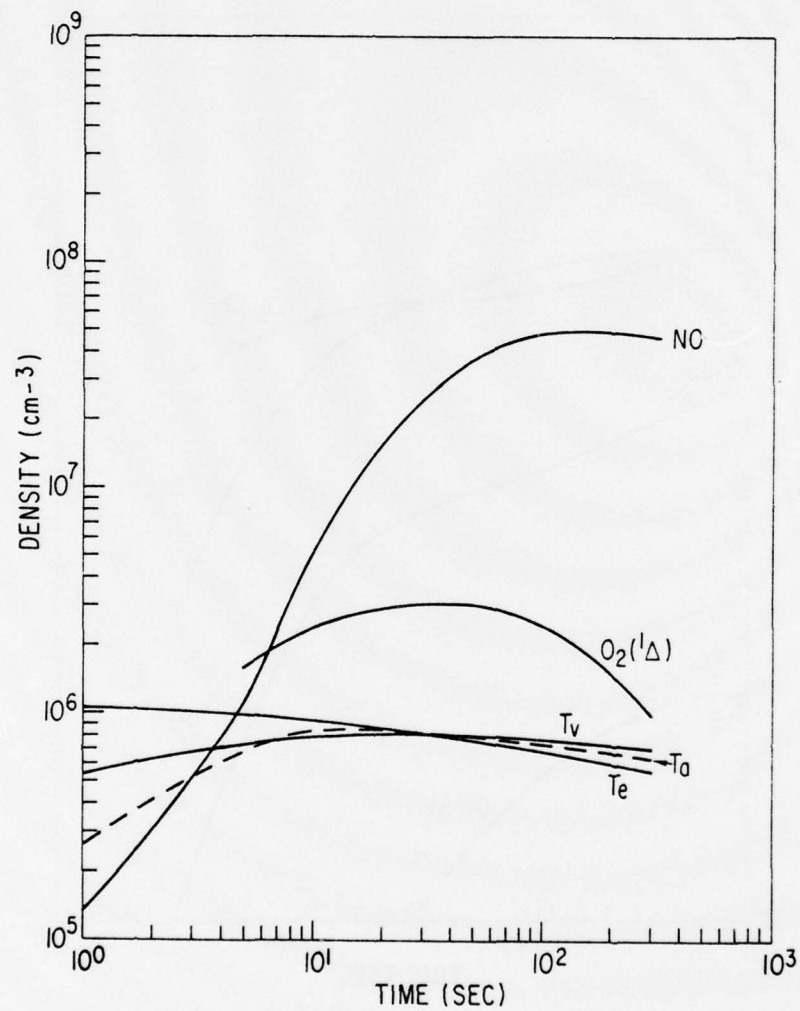


Fig. 5 - The time history of NO,  $\text{O}_2(^1\Delta)$ ,  $T_v$ ,  $T_a$  and  $T_e$  for Case I

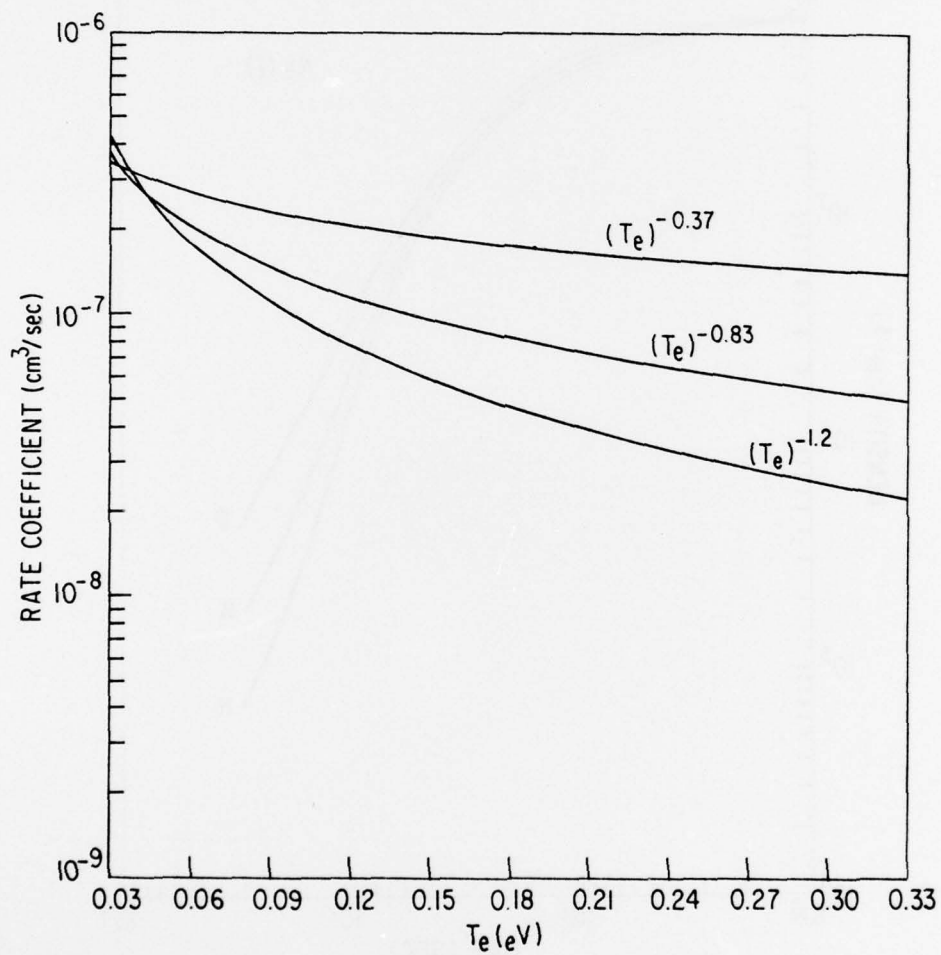


Fig. 6 - The dissociative recombination rate coefficient of  $\text{NO}^+$  as a function of the electron temperature

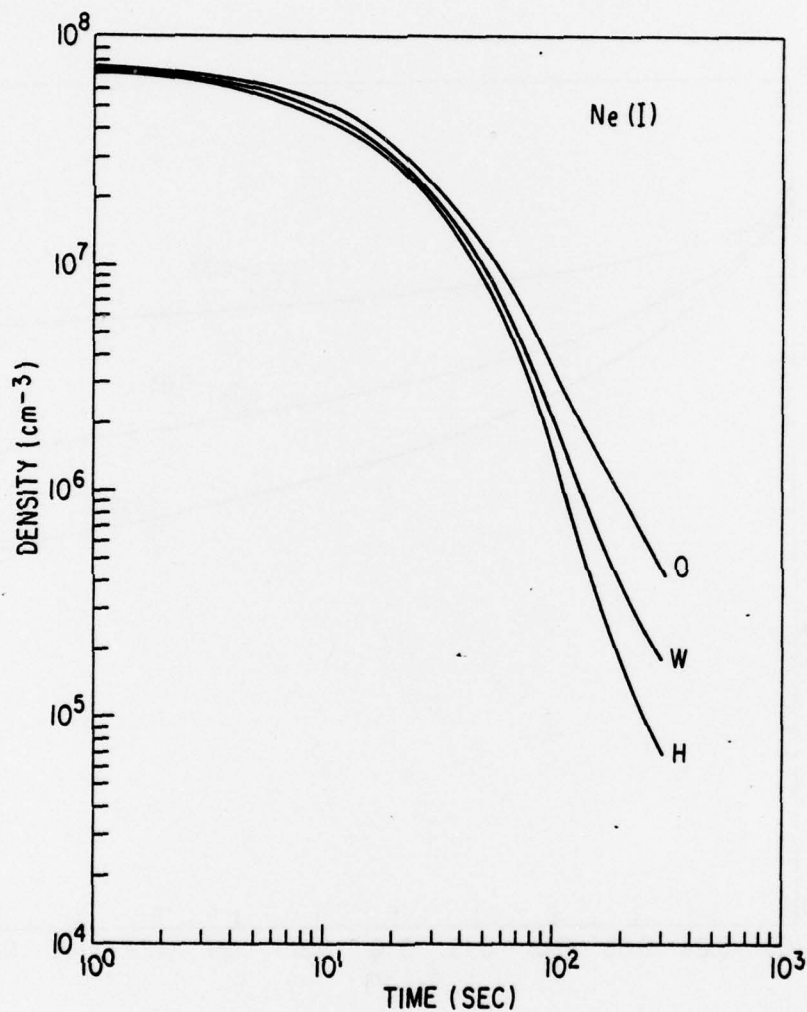


Fig. 7 - The electron density for Case I as a function of time using the  $\text{NO}^+$  dissociative recombination rate coefficients of Fig. 6. The notations O, W and H stand for O (old Ref. 5), W (Walls and Dunn Ref. 10) and H (Huang, et al, Ref. 9), respectively. The temperature dependence of these rates are  $O \sim T_e^{-1.2}$ ,  $W \sim T_e^{-0.83}$  and  $H \sim T_e^{-0.37}$ , respectively.



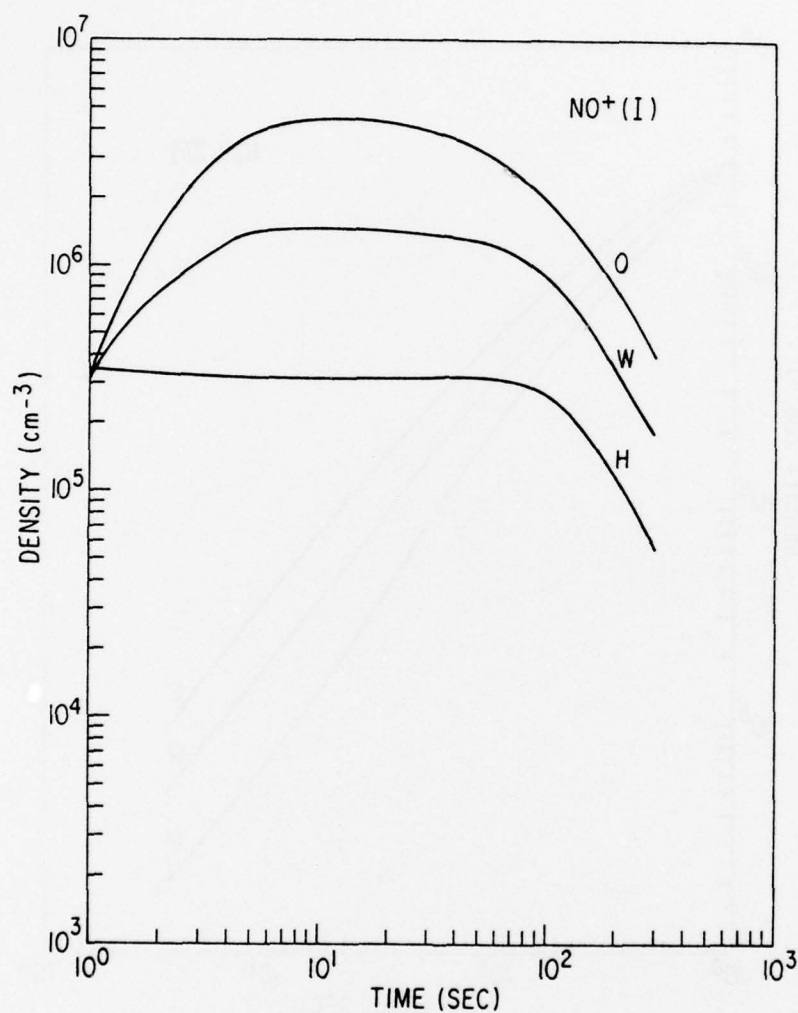


Fig. 8 - The NO<sup>+</sup> density for Case I using rate coefficients of Fig. 6. The notations O, W and H are described in the caption of Fig. 7.

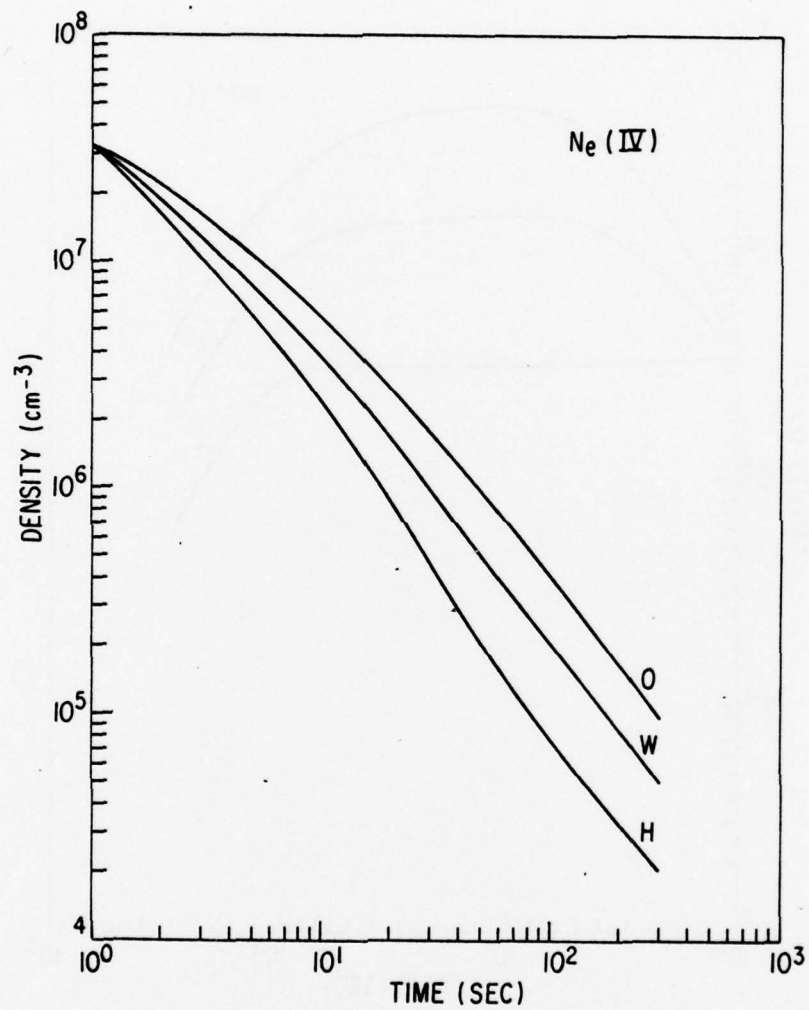


Fig. 9 - The electron density for Case IV using the dissociative recombinations of Fig. 6

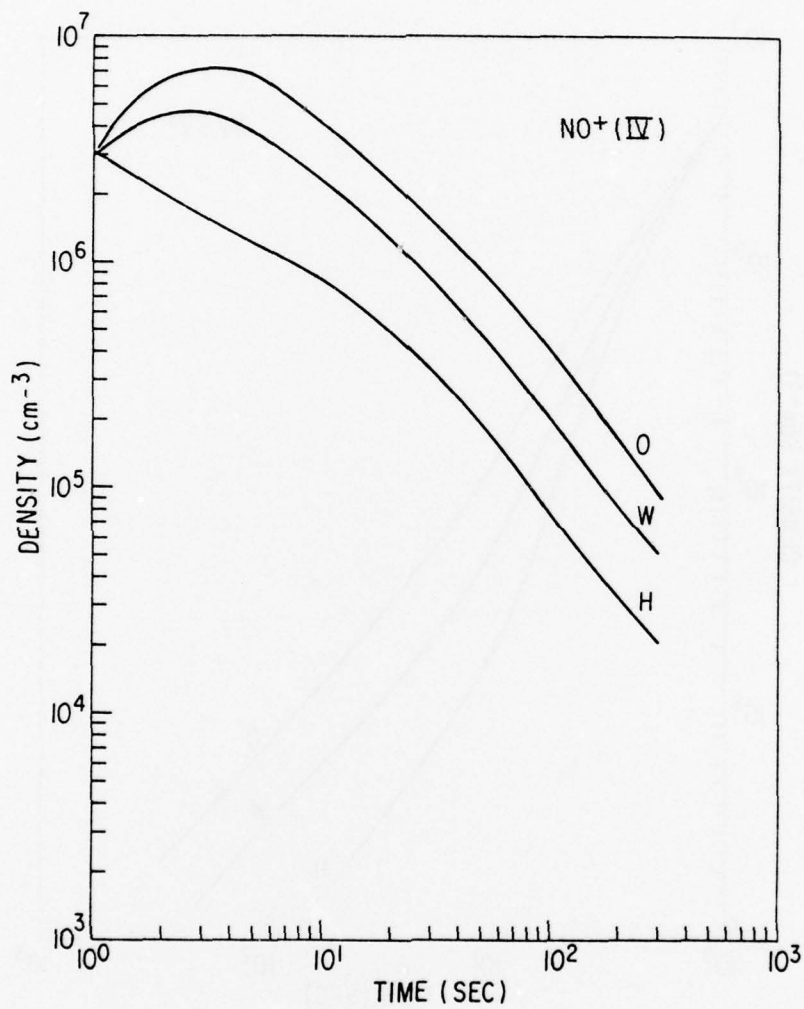


Fig. 10 - The NO<sup>+</sup> density for Case IV using the dissociative recombinations of Fig. 6

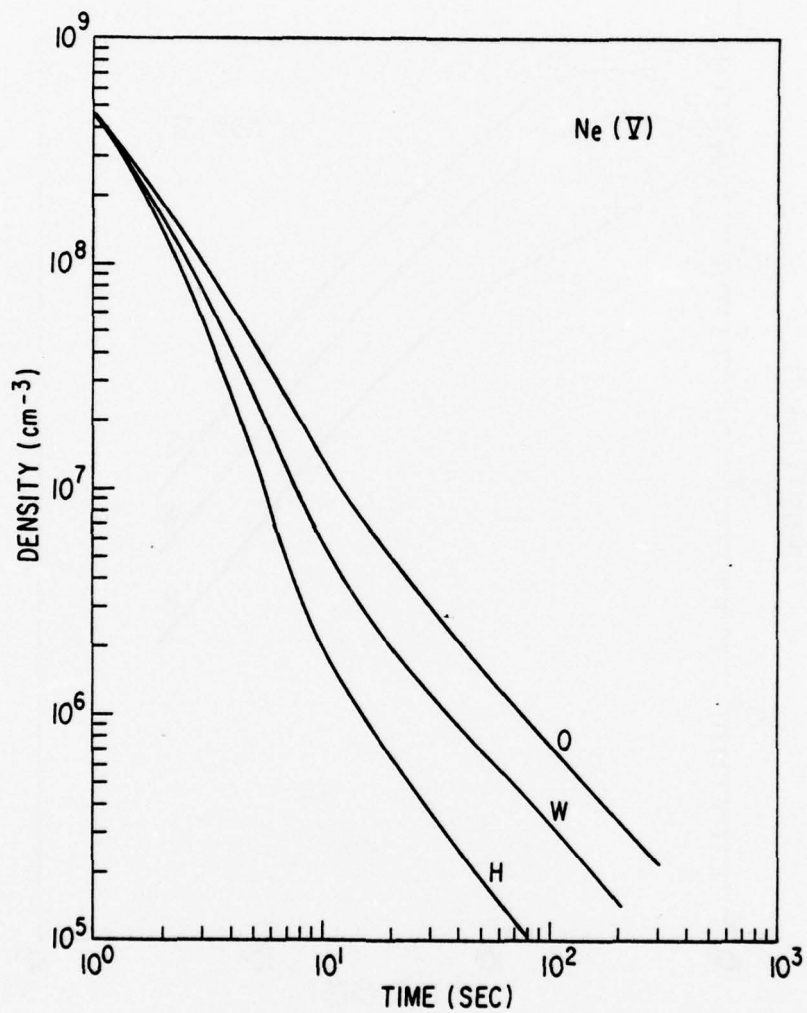


Fig. 11 - The electron density for Case V using the dissociative recombination rates of Fig. 6

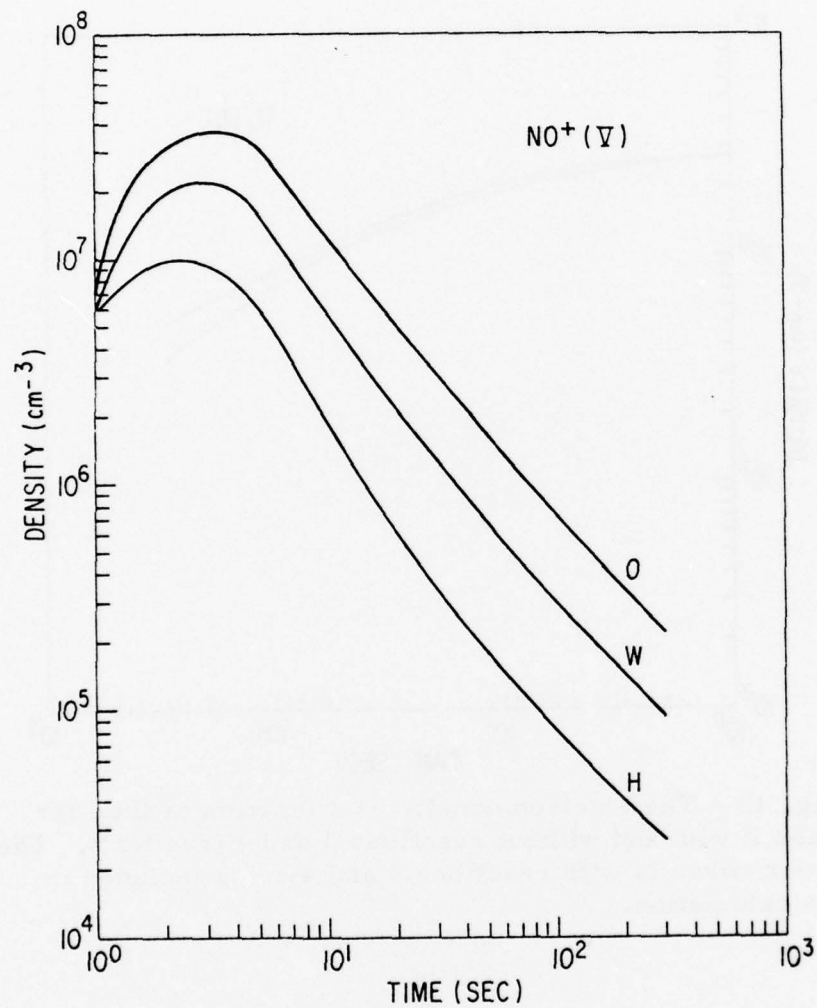


Fig. 12 - The NO<sup>+</sup> density for Case V using the dissociative recombination rates of Fig. 6

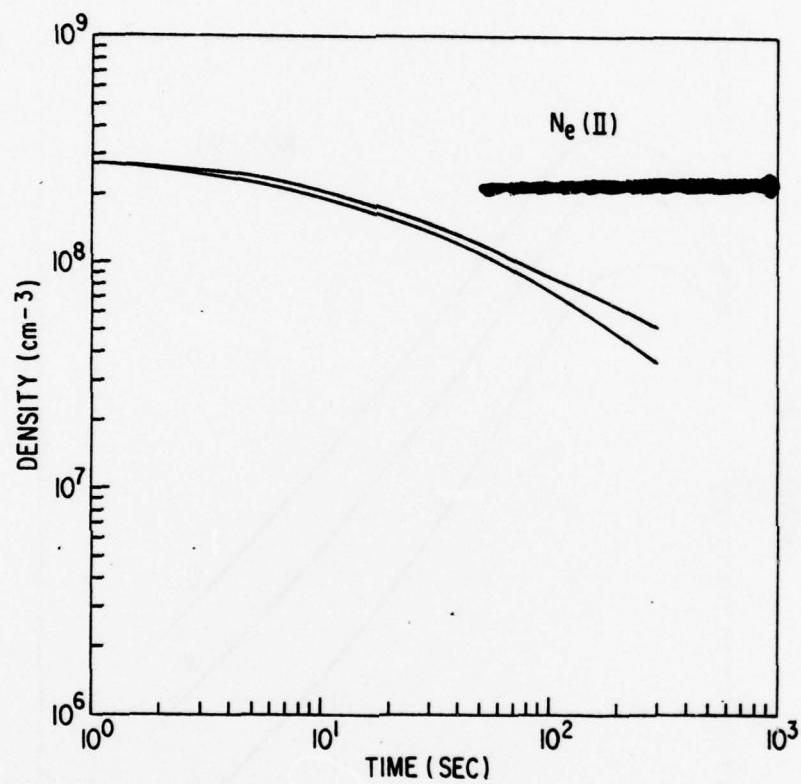


Fig. 13 - The electron density as a function of time for Case II with and without reactions 3 and 4 (see text). The lower curve is with reactions 3 and 4 being included in the calculation.



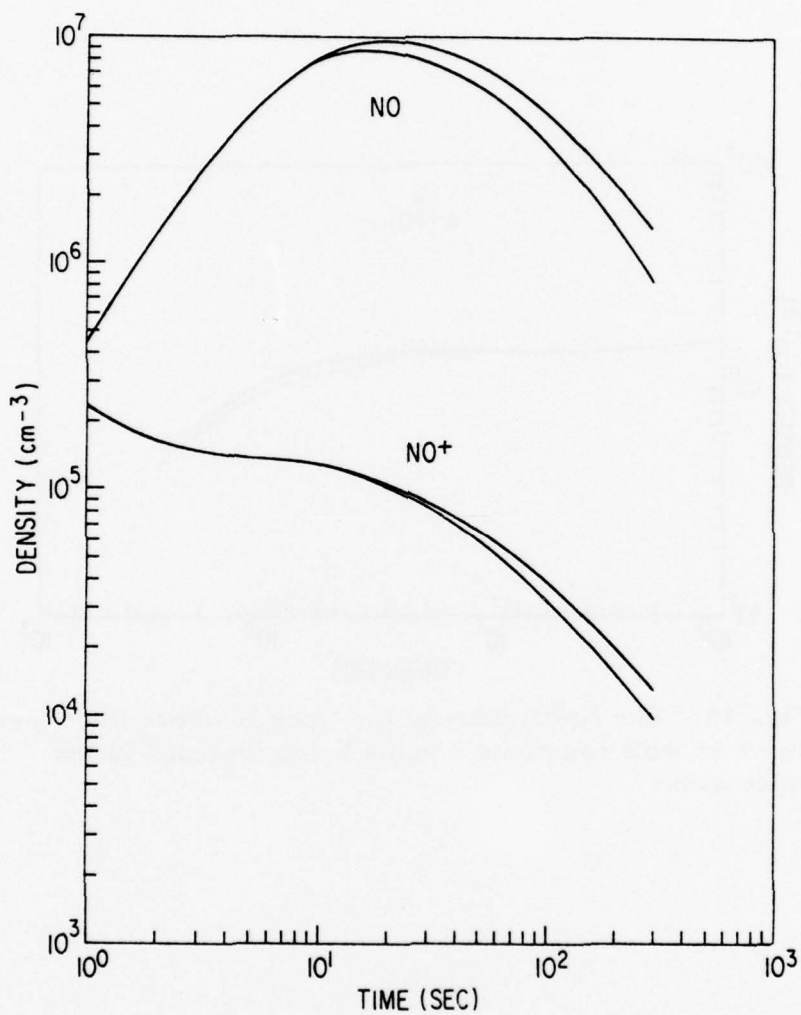


Fig. 14 - The NO and NO<sup>+</sup> densities for Case II with and without reactions 3 and 4 (see text). The upper curves are with reactions 3 and 4 being included in the calculation.

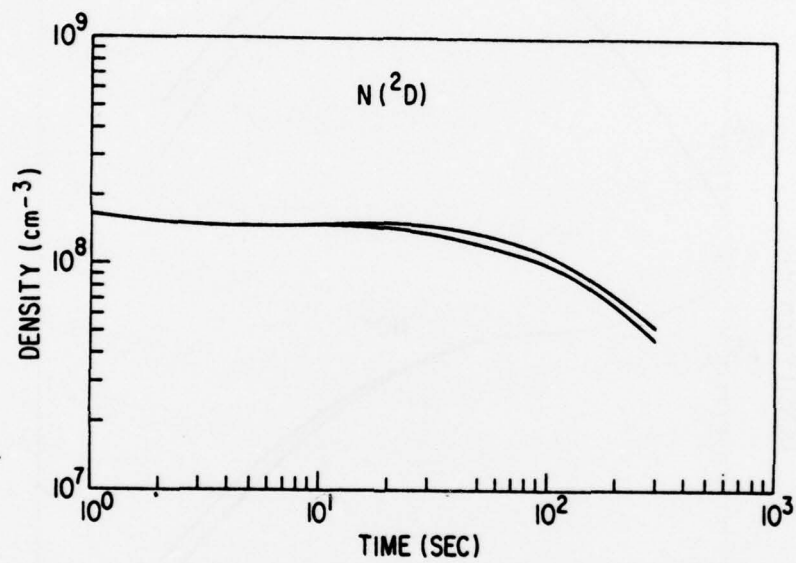


Fig. 15 - The  $N(^2D)$  density for Case II where the upper curve is with reactions 3 and 4 being included in the calculation

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